

Welcome to STN International! Enter x:x

LOGINID:ssspta1611sxp

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
NEWS 3 Jun 03 New e-mail delivery for search results now available  
NEWS 4 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 5 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)  
now available on STN  
NEWS 6 Aug 26 Sequence searching in REGISTRY enhanced  
NEWS 7 Sep 03 JAPIO has been reloaded and enhanced  
NEWS 8 Sep 16 Experimental properties added to the REGISTRY file  
NEWS 9 Sep 16 CA Section Thesaurus available in CAPLUS and CA  
NEWS 10 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985  
NEWS 11 Oct 24 BEILSTEIN adds new search fields  
NEWS 12 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN  
NEWS 13 Nov 18 DKILIT has been renamed APOLLIT  
NEWS 14 Nov 25 More calculated properties added to REGISTRY  
NEWS 15 Dec 04 CSA files on STN  
NEWS 16 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date  
NEWS 17 Dec 17 TOXCENTER enhanced with additional content  
NEWS 18 Dec 17 Adis Clinical Trials Insight now available on STN  
NEWS 19 Jan 29 Simultaneous left and right truncation added to COMPENDEX,  
ENERGY, INSPEC  
NEWS 20 Feb 13 CANCERLIT is no longer being updated  
NEWS 21 Feb 24 METADEX enhancements  
NEWS 22 Feb 24 PCTGEN now available on STN  
NEWS 23 Feb 24 TEMA now available on STN  
NEWS 24 Feb 26 NTIS now allows simultaneous left and right truncation  
NEWS 25 Feb 26 PCTFULL now contains images  
NEWS 26 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results  
NEWS 27 Mar 19 APOLLIT offering free connect time in April 2003  
NEWS 28 Mar 20 EVENTLINE will be removed from STN  
NEWS 29 Mar 24 PATDPAFULL now available on STN  
NEWS 30 Mar 24 Additional information for trade-named substances without  
structures available in REGISTRY  
NEWS 31 Apr 11 Display formats in DGENE enhanced  
NEWS 32 Apr 14 MEDLINE Reload  
NEWS 33 Apr 17 Polymer searching in REGISTRY enhanced  
NEWS 34 Apr 21 Indexing from 1947 to 1956 being added to records in CA/CAPLUS  
NEWS 35 Apr 21 New current-awareness alert (SDI) frequency in  
WPIDS/WPINDEX/WPIX  
NEWS 36 Apr 28 RDISCLOSURE now available on STN  
  
NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT  
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003  
NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS INTER      General Internet Information  
NEWS LOGIN      Welcome Banner and News Items  
NEWS PHONE      Direct Dial and Telecommunication Network Access to STN  
NEWS WWW        CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 10:43:28 ON 03 MAY 2003

=> ile reg

ILE IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.  
For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:43:42 ON 03 MAY 2003

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES:    2 MAY 2003    HIGHEST RN 509953-09-7  
DICTIONARY FILE UPDATES:   2 MAY 2003    HIGHEST RN 509953-09-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when

conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

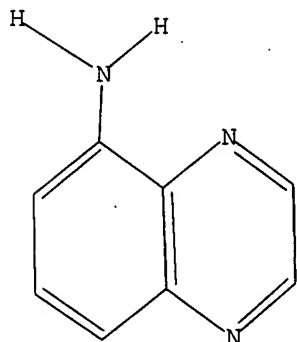
Uploading 10077150.2

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 10:43:57 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 298 TO ITERATE

100.0% PROCESSED 298 ITERATIONS

19 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 4925 TO 6995

PROJECTED ANSWERS: 119 TO 641

L2 19 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 10:44:06 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5624 TO ITERATE

100.0% PROCESSED 5624 ITERATIONS

311 ANSWERS

SEARCH TIME: 00.00.01

L3 311 SEA SSS FUL L1

=&gt; file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

148.15

148.36

FILE 'CAPLUS' ENTERED AT 10:44:12 ON 03 MAY 2003

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FILE COVERS 1907 - 3 May 2003 VOL 138 ISS 19

FILE LAST UPDATED: 2 May 2003 (20030502/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=&gt; s 13

L4 261 L3

=&gt; s 14 and pyrimidine

L5 5 L4 AND PYRIMIDINE

=&gt; s 14 and diaminipyrimidine

L6 0 L4 AND DIAMINIPYRIMIDINE

=&gt; d 15 fbib hitstr abs total

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS

AN 1997:618093 CAPLUS

DN 127:293249

TI Preparation of quinoxalinediones as NMDA receptor antagonists

IN Bull, David John; Carr, Christopher Lee; Fray, Michael Jonathan; Gautier, Elisabeth Colette Louise; Mowbray, Charles Eric; Stobie, Alan

PA Pfizer Research and Development Company, N.V., UK; Pfizer Inc.; Bull, David John; Carr, Christopher Lee; Fray, Michael Jonathan; Gautier, Elisabeth Colette Louise; Mowbray, Charles Eric; Stobie, Alan

SO PCT Int. Appl., 153 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9732873	A1	19970912	WO 1997-EP995	19970227

W: AU, BG, BR, CA, CN, CZ, HU, IL, IS, JP, KR, LK, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ,

MD, RU, TJ, TM  
 RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT,  
 SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

TW 454004	B	20010911	GB 1996-5027 A 19960309
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CA 2248366	AA	19970912	GB 1996-5027 A 19960309
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AU 9720231	A1	19970922	GB 1996-5027 A 19960309
AU 717972	B2	20000406	AU 1997-20231 19970227
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NO 9904135	A	19991022	US 1999-367303		19990802
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## PATENT FAMILY INFORMATION:

FAN 1998:608616

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PI	WO 9838186	A1	19980903	WO 1998-EP1275		19980224
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
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US 6333326 B1 20011225

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OS MARPAT 127:293249

IT 178619-88-0P 178619-89-1P 178907-46-5P

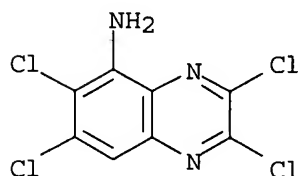
178907-47-6P 178907-48-7P 178907-49-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of quinoxalinediones as NMDA receptor antagonists)

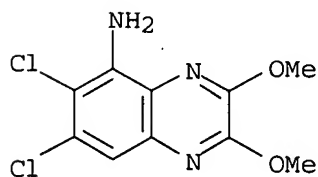
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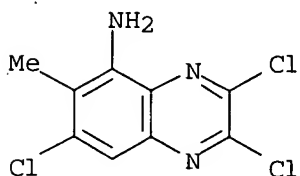
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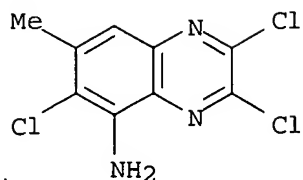
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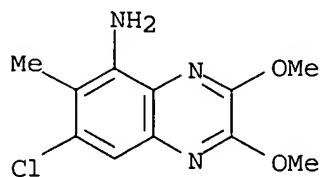
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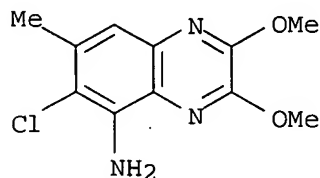
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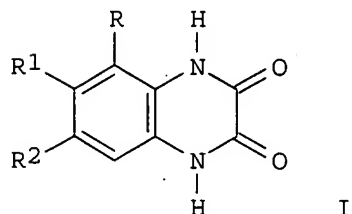


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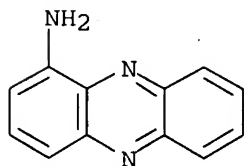
GI



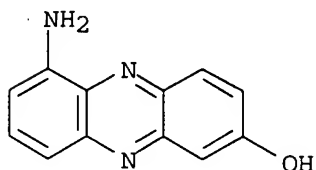
AB The title compds. [I; R = (un)substituted 5-membered heteroaryl contg. 3 or 4 N atoms which is linked to the quinoxalinedione ring by a ring C or N atom, or a 6-membered heteroaryl contg. 1-3 N atoms which is linked to the quinoxalinedione ring by a ring C atom; R1, R2 = H, F, Cl, C1-4 alkyl, etc.], useful as NMDA receptor antagonists for treating acute neurodegenerative and chronic neurol. disorders such as stroke, transient ischemic attack, peri-operative ischemia or traumatic head injury, were prepd. and formulated. Thus, treatment of 6,7-dichloro-2,3-dimethoxy-5-(4-pyridyl)quinoxaline with 2N HCl in 1,4-dioxane afforded 17% I [R = 4-pyridyl; R1 = R2 = H]. Compd. I [R = 1-methyl-1H-tetrazol-5-yl; R1 = R2 = Cl] showed IC50 of 3 nM against binding at the glycine site of the NMDA

receptor.

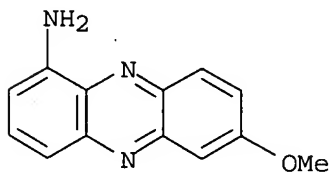
L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS  
AN 1963:53246 CAPLUS  
DN 58:53246  
OREF 58:9060h,9061a-g  
TI Phenazines. II. Synthesis of aminophenazines  
AU Gaertner, G.; Gray, A.; Holliman, F. G.  
CS Univ. Cape Town, S. Afr.  
SO Tetrahedron (1962), 18, 1105-14  
DT Journal  
LA Unavailable  
IT 2876-22-4, Phenazine, 1-amino- 18450-04-9, 2-Phenazinol,  
6-amino- 18450-05-0, Phenazine, 1-amino-7-methoxy-  
92164-56-2, 2-Phenazinol, 6-amino-, acetate  
(prepn. of)  
RN 2876-22-4 CAPLUS  
CN 1-Phenazinamine (9CI) (CA INDEX NAME)



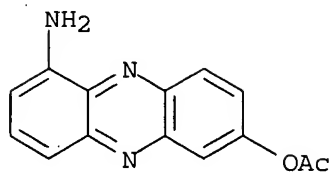
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RN 18450-05-0 CAPLUS  
CN Phenazine, 1-amino-7-methoxy- (7CI, 8CI) (CA INDEX NAME)



RN 92164-56-2 CAPLUS  
CN 2-Phenazinol, 6-amino-, acetate (7CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB Polynitrodiphenylamines (I) were prepd. by Ullmann reactions under a variety of conditions as detailed in tabulation. The appropriate I were catalytically hydrogenated in alc. with prereduced PtO<sub>2</sub> or Pd-C at 20-40 lb./sq. in. and the filtered soln. was evapd. (N atm) in vacuo to give the corresponding aminodiphenylamines (II), characterized as the polyacetamido derivs. (R, R<sub>1</sub>, R<sub>2</sub>, R<sub>3</sub>, R<sub>4</sub>, and m.p. (solvent) given): MeO, AcNH, H, AcNH, H, AcNH, H, 215.0-6.5.degree. (BuOH); H, MeO, AcNH, AcNH, AcNH, H, 238-40.degree. (PhNO<sub>2</sub>); H, AcNH, MeO, H, AcNH, H, 202-4.degree. (alc.); Me, AcNH, H, H, AcNH, H, 232-4.degree. (dil. alc.); Cl, AcNH, H, H, AcNH, H, 239-41.degree. (dil. alc.). Only II(R = H, R<sub>1</sub> = R<sub>2</sub> = NH<sub>2</sub>, R<sub>3</sub> = MeO, R<sub>4</sub> = H), m. 155-8.degree. (alc.-Norit), was analyzed directly. II (R = MeO, R<sub>1</sub> = R<sub>3</sub> = R<sub>5</sub> = NH<sub>2</sub>, R<sub>2</sub> = R<sub>4</sub> = H) from catalytic hydrogenation of 2 g. I in alc. treated with 10 ml. 6N HCl and filtered (N atm.) from catalyst, the filtrate dild. with 6.6 g. FeCl<sub>3</sub> in 32 ml. H<sub>2</sub>O and the mixt. kept 1 day, the alc. evapd. and the residue adjusted to pH 5-6 with NaOAc gave 75% 1-amino-7-methoxyphenazine (III, R = NH<sub>2</sub>, R<sub>3</sub> = MeO, R<sub>1</sub> = R<sub>2</sub> = R<sub>4</sub> = H) (IV), m. 168-71.degree. (ligroine b. 80-100.degree.). IV (0.2 g.) in 4.5 ml. 48% HBr refluxed 3 hrs. and the cooled mixt. made alk., the filtered soln. adjusted to pH 6 with HCl and filtered, the H<sub>2</sub>O-washed ppt. crystd. from H<sub>2</sub>O and dried in vacuo over CaCl<sub>2</sub> gave III (R = NH<sub>2</sub>, R<sub>3</sub> = OH, R<sub>1</sub> = R<sub>2</sub> = R<sub>4</sub> = H) (V), m. 270.degree. (decompn.), acetylated with Ac<sub>2</sub>O at 20.degree. to give III (R = NHAc, R<sub>3</sub> = OH, R<sub>1</sub> = R<sub>2</sub> = R<sub>4</sub> = H) m. 297.degree. (decompn.). V acetylated at 0.degree. with Ac<sub>2</sub>O in the presence of aq. NaOH gave III (R<sub>1</sub> = AcO, R<sub>2</sub> = NH<sub>2</sub>, R = R<sub>3</sub> = R<sub>4</sub> = H), m. 182-5.degree. (alc.), hydrolyzed in warm dil. alkali with formation of a deep red soln. V acetylated by heating with Ac<sub>2</sub>O and NaOAc gave III (R = NHAc, R<sub>3</sub> = AcO, R<sub>1</sub> = R<sub>2</sub> = R<sub>4</sub> = H), m. 205-8.degree. (alc.). II obtained from 1 g. of the corresponding nitro compd. refluxed 1 hr. in 50-60 ml. xylene with 15 g. PbO<sub>2</sub> and the filtered soln. and washings extd. with 6N HCl, the acid ext. neutralized and the product recrystd. gave the tabulated III (I and III substituents other than H, m.p. III (solvent) and % yield given): R<sub>1</sub> = R<sub>4</sub> = NO<sub>2</sub>, R<sub>1</sub> = NH<sub>2</sub>, 274-7.degree. (dil. alc.), -(low); R = R<sub>1</sub> = NO<sub>2</sub>, R<sub>1</sub> = NH<sub>2</sub>, 265-70.degree. (alc.), 13; R<sub>1</sub> = R<sub>3</sub> = NO<sub>2</sub>, R<sub>1</sub> = NH<sub>2</sub>, 115-40.degree., -(low); R = R<sub>1</sub> = NO<sub>2</sub>, R<sub>4</sub> = MeO, R<sub>1</sub> = NH<sub>2</sub>, R<sub>4</sub> = MeO, 212-15.degree. (H<sub>2</sub>O), -(low); R<sub>1</sub> = R<sub>2</sub> NO<sub>2</sub>, R<sub>3</sub> = MeO, R = NH<sub>2</sub>, 169-72.degree. (H<sub>2</sub>O), 43; R<sub>1</sub> = NO<sub>2</sub>, R = NH<sub>2</sub>, 169-71.degree. (sublimation), -(low). II (obtained by evapn. of filtered hydrogenation alc. soln.) refluxed 5 hrs. in 25 ml. PhNO<sub>2</sub> contg. 0.5 g. m-(O<sub>2</sub>N)<sub>2</sub>C<sub>6</sub>H<sub>4</sub> and dild. with 100 ml. 6N HCl, the mixt. steam distd. and the acid residue neutralized gave III (method A). II (catalysts soln. after filtration) dild. with 125 ml. PhNO<sub>2</sub> and the alc. evapd., the PhNO<sub>2</sub> soln. refluxed 12 hrs. and the soln. concd. in vacuo to 25 ml., the concentrate cooled and filtered yielded III (method B). Phys. data are tabulated (substituents of I other than H, method, substituents of III other than H, m.p. (solvent) and % yield given): R<sub>2</sub> = R<sub>4</sub> = NO<sub>2</sub>, R<sub>1</sub> = MeO, A, R<sub>1</sub> = NH<sub>2</sub>, R<sub>2</sub> = MeO, 278-81.degree. (H<sub>2</sub>O), 44; R<sub>1</sub> = R<sub>4</sub> = NO<sub>2</sub>, A, R<sub>1</sub> = NH<sub>2</sub>, 277-80.degree. (50% alc.), 50; R = R<sub>1</sub> = NO<sub>2</sub>, A, R<sub>1</sub> = NH<sub>2</sub>, 277-80.degree. (50% alc.), 5; R = R<sub>1</sub> = NO<sub>2</sub>, B, R<sub>1</sub> = NH<sub>2</sub>, 270-4.degree. (50% alc.), 50; R = R<sub>1</sub> = NO<sub>2</sub>, R<sub>4</sub> = MeO, A, R<sub>1</sub> = NH<sub>2</sub>, R<sub>4</sub> = MeO, 216-18.degree. (H<sub>2</sub>O), 54; R<sub>4</sub> = Me, R = R<sub>1</sub> = NO<sub>2</sub>, B,

R1 = NH<sub>2</sub>, R4 = Me, 228-30.degree. (dil. alc.), 52; R = Me, R1 = R4 = NO<sub>2</sub>, B, R1 = NH<sub>2</sub>, R4 = Me, 228-30.degree. (dil. alc.), 46; R = R1 = NO<sub>2</sub>, R4 = Cl, B, R1 = NH<sub>2</sub>, R4 = Cl, 250-1.degree. (dil. alc.), 45; R = Cl, R1 = R4 = NO<sub>2</sub>, B, R1 = NH<sub>2</sub>, R4 = Cl, 247-9.degree. (dil. alc.), 30; R1 = R3 = NO<sub>2</sub>, A, R = NH<sub>2</sub>, 174-6.degree. (dil. alc.), 67; R1 = R2 = NO<sub>2</sub>, A, R = NH<sub>2</sub>, 174-6.degree. (dil. alc.), 25; R1 = R2 = NO<sub>2</sub>, R3 = MeO, A, R = NH<sub>2</sub>, 123-8.degree. (crude, identified by paper chromatography), small. Ultraviolet and visible spectral data, and fluorescence data were given.

L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2003 ACS

AN 1963:3286 CAPLUS

DN 58:3286

OREF 58:521d-f

TI Polyazanaphthalenes. VII. Some derivatives of quinazoline and 1,3,5-triazanaphthalene

AU Oakes, V.; Rydon, H. N.; Undheim, K.

CS Univ. Exeter, UK

SO J. Chem. Soc. (1962) 4678-85

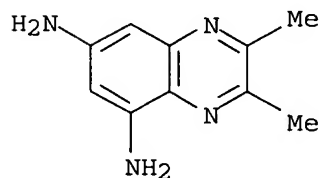
DT Journal

LA Unavailable

IT 2312-92-7, Quinoxaline, 5,7-diamino-2,3-dimethyl-  
89977-47-9, Quinoxaline, 5,7-diamino- 90558-60-4,  
Quinoxaline, 6,8-diamino-2-methyl- 90558-76-2, 2-Quinoxalinol,  
5,7-diamino-3-methyl- 91769-37-8, 2-Quinoxalineacetic acid,  
6,8-diamino-3-hydroxy-, ethyl ester  
(prepn. of)

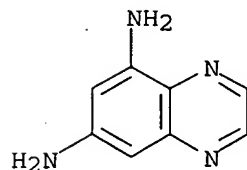
RN 2312-92-7 CAPLUS

CN 5,7-Quinoxalinediamine, 2,3-dimethyl- (9CI) (CA INDEX NAME)



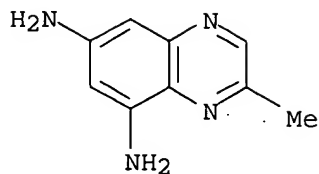
RN 89977-47-9 CAPLUS

CN Quinoxaline, 5,7-diamino- (7CI) (CA INDEX NAME)



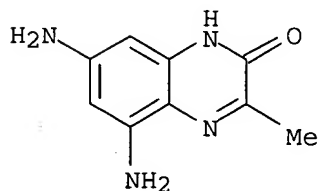
RN 90558-60-4 CAPLUS

CN Quinoxaline, 6,8-diamino-2-methyl- (7CI) (CA INDEX NAME)



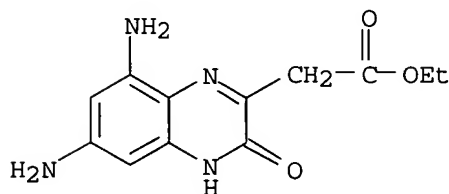
RN 90558-76-2 CAPLUS

CN 2-Quinoxalinol, 5,7-diamino-3-methyl- (7CI) (CA INDEX NAME)



RN 91769-37-8 CAPLUS

CN 2-Quinoxalineacetic acid, 6,8-diamino-3-hydroxy-, ethyl ester (7CI) (CA INDEX NAME)



GI For diagram(s), see printed CA Issue.

AB 2,4-Diamino-6-methylquinazoline was synthesized and converted, by side-chain bromination of its dibenzoyl deriv., condensation with ethyl p-aminobenzoate, and removal of the benzoyl and ester groups, into the pteric acid analog (I). A similar procedure has led to the successful synthesis of pteric acid analogs derived from 2,4-diamino- and 2-amino-4-hydroxy-1,3,5-triazanaphthalene. The expected preferential reactivity of the 4-chlorine atom in 2,4-dichloro-6-methylquinazoline is exhibited in its reactions with ammonia, hydrazine, and benzylamine, but not in that with aniline.

L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS

AN 1962:13016 CAPLUS

DN 56:13016

OREF 56:2449d-g

TI 5-Ethoxy-8-aminoquinoxaline

AU Easley, Wm. K.; Monley, Lawrence E.; Hutchins, James E.

CS Northern Louisiana State Coll., Monroe

SO J. Org. Chem. (1961), 26, 3008-9

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

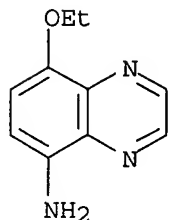
LA Unavailable

IT 90840-14-5, Quinoxaline, 5-amino-8-ethoxy- 93439-84-0,

Quinoxaline, 5-amino-8-ethoxy-, hydrochloride  
(prepn. of)

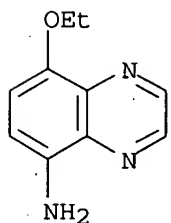
RN 90840-14-5 CAPLUS

CN Quinoxaline, 5-amino-8-ethoxy- (7CI) (CA INDEX NAME)



RN 93439-84-0 CAPLUS

CN Quinoxaline, 5-amino-8-ethoxy-, hydrochloride (7CI) (CA INDEX NAME)



x HCl

AB The synthesis of 5-ethoxy-8-(acetylamino)quinoxaline (I), 5-ethoxy-8-aminoquinoxaline (II), 5-ethoxy-8-(p-toluenesulfonamido)quinoxaline (III), 5-ethoxy-8-(N-acetylsulfanilamido)quinoxaline (IV), and 5-ethoxy-8-sulfanil-amidoquinoxaline (V) was reported together with an improved procedure for 1-ethoxy-2,3-dinitro-4-acetamido-benzene (VI). p-Phenacetin (25 g.) treated during 1 hr. at 15-25.degree. with 125 ml. fuming HNO<sub>3</sub>, the mixt. poured into 1.5 l. cold H<sub>2</sub>O, and the product crystd. gave 28.1 g. VI, plates, m. 211-12.degree.. The av. yield of VI from 14 similar runs was 75%. VI (54 g.) in 350 ml. HCONMe<sub>2</sub> reduced in the presence of 40 g. 5% Pd-C at room temp./30 lb./sq. in. 1.5 hrs., the mixt. filtered under N into 68.1 g. Na glyoxal bisulfite in 1 l. 70.degree. H<sub>2</sub>O, refluxed 6 hrs. under N, filtered, the filtrate evapd., and the oil poured into 31. Me<sub>2</sub>CO gave 21.3 g. I, m. 186.degree.. I (2 g.) and 20 ml. 2NH<sub>2</sub>SO<sub>4</sub> heated 15 min. at 95-8.degree., the soln. cooled, neutralized, and the solid washed and recrystd. gave 1.48 g. II, m. 85-6.degree. (alc.-Me<sub>2</sub>CO). II appeared to undergo a no. of the usual reactions of aromatic amines. It could be coupled with .beta.-naphthol, 1-phenyl-3-methyl-5-pyrazolone, p-cresol, di-phenylamine, dimethylaniline, and N-ethyl-N-(.beta.-cyano-ethyl)-m-toluidine to form dyes. II (0.5 g.) in 10 ml. alc. stirred 1 hr. at room temp. with excess 14% HCl gave 0.59g. II.HCl, m. 180-90.degree.. p-MeC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>Cl (0.33 g.) refluxed 0.5 hr. with 0.5 g. II gave 0.48 g. III, m. 132-3.degree. (alc.-Me<sub>2</sub>CO). IV was obtained in 90.5% yield, m. 223-9.degree.. Alc. HCl hydrolysis of IV gave 71% V, yellow, m.

181-2.degree..

L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS

AN 1958:55935 CAPLUS

DN 52:55935

OREF 52:10095e-i,10096a-i,10097a-g

TI Aminoisoquinolines, -cinnolines, and -quinazolines. (A) The basic strengths and ultraviolet absorption spectra. (B) Infrared spectra

AU Osborn, A. R.; Schofield, K.; Short, L. N.

CS Washington Singer Labs., Exeter, UK

SO J. Chem. Soc. (1956) 4191-206

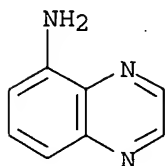
DT Journal

LA Unavailable

IT 16566-20-4, Quinoxaline, 5-amino-  
(basicity and spectra of)

RN 16566-20-4 CAPLUS

CN 5-Quinoxalinamine (9CI) (CA INDEX NAME)



AB cf. following abstr. Potentiometric titrations in aq. soln. at 20.degree. with HCl gave the following pKa values. Isoquinolines: unsubstituted (I), 5.40; 3-NH2 (Ia), 5.05; 4-NH2 (Ib), 6.28; 5-NH2 (Ic), 5.59; 6-NH2 (Id), 7.17; 7-NH2 (Ie), 6.20; 8-NH2 (If), 6.06. Cinnolines: unsubstituted (II), 2.29; 3-NH2 (IIa), 3.70; 4-NH2 (IIb), 6.85; 5-NH2 (IIc), 2.70; 6-NH2 (IId), 5.04; 7-NH2 (IIe), 4.85; 8-NH2 (IIIf), 3.68. Quinazolines: unsubstituted (III), 3.51; 2-NH2 (IIIa), 4.82; 4-NH2 (IIIb), 5.85; 5-NH2 (IIIc), 3.57; 6-NH2 (IIId), 3.29; 7-NH2 (IIIe), 4.60; 8-NH2 (IIIIf), 2.81. In addn. pKa values based on calcns. from ultraviolet extinction curves were detd. for phenanthridine 4.52, its 6-NH2 deriv. 6.88, and 6,7-benzoquinazoline (IV) .apprx. 5.2. Ultraviolet absorption data for the above bases and their cations in buffered aq. solns. and of the methochlorides of I, II, and III in H2O were given. I, II, and III showed the 3 main bands characteristic of electronic transitions parallel to the long, short, and long axes of bicyclic systems, and the effect of the position of the NH2 substituent could be correlated fairly well with the shifts of the bands noted in the spectra of their NH2 derivs. II in cyclohexane showed an addnl. low-intensity, longer wavelength (390 m.mu.) band of an n .fwdarw. .pi. transition which disappeared in water or acid. The bathochromic shift shown in the spectra of the aminoisoquinolines on conversion to the cations indicated that, as with I, the monocations carry the proton on the ring N. Study of the .DELTA.pKa values (relative to I) showed values below 1 for Ib, Ic, and Ie, in which there is no possibility of addnl. ionic resonance in the cations, and above 1 for the 1-NH2 deriv. of I and Id, for which addnl. forms are possible, and a neg. value for Ia, which is clearly not increased in stability by a possible .omicron.-quinonoid resonance form (see the following abstr. for If). The bathochromic shifts in the spectra of the aminocinnolines on cation formation again indicated that proton attachment is to the ring N. By analogies to the quinoline and isoquinoline series; .DELTA.pKa values indicated that N1 is the predominant basic center in IIb, IIe, and

probably IIc, while N2 is the basic center for IIId and IIIf (the spectra of If and IIIf are similar). From the values of  $\Delta pK_a$  for IIa, the basic center is considered to be N2, although it contrasts strongly with Ia. Cationization of III caused a marked hypsochromic shift in contrast to the more usual slight bathochromic shift for other heterocyclic bases, and some modification of the aromatic system, possibly a 3,4-hydration, is assumed. Ultraviolet studies on cation formation of the aminoquinazolines indicated no hydration for IIIa and IIIb (similar to 2- and 4-aminoquinoline), IIIc, IIIe, and IIIf, while IIId is presumably hydrated. Considering the change on cationization of III and the increased base strength of 3,4-dihydroquinazolines relative to the quinazolines, choice of a basic center by correlation with  $\Delta pK_a$  values is difficult, although N1 seems to be favored for IIIb and definite for IIIe. Quinoxaline and its 6-NH<sub>2</sub> deriv. also showed the usual bathochromic shift on cation formation, while the 5-NH<sub>2</sub> deriv. seemed to take up the first proton on its NH<sub>2</sub> group. Infrared N-H bond stretching frequencies and force constants, indicative of the amt. of interaction of the NH<sub>2</sub> group with the ring and the electron density at the ring N, were given for Ia-f, IIa-f, IIIa-f, 2-, 4-, and 5-aminopyrimidines, and 5-aminoquinoline in CCl<sub>4</sub>, CHCl<sub>3</sub>, and pyridine (some compds.); the effects of electromeric interaction where possible, the lack of interaction between N1 and a C-5 NH<sub>2</sub> group, the effect of 2 ring N atoms adjacent to the NH<sub>2</sub> group and of intramolecular H-bonding were noted.

1,3-Dichloroisoquinoline (0.5 g.), 25 cc. MeOH, 0.4 g. KOH, and 3 cc. Raney Ni shaken with H, the MeOH evapd., and the Et<sub>2</sub>O ext. of the residue treated with picric acid in Et<sub>2</sub>O gave I picrate, m. 225-6.degree.; 1,3-dibromoisoquinoline (V) behaved similarly. Homophthalimide (5 g.) and 50 cc. PBr<sub>3</sub> refluxed 5 hrs., the PBr<sub>3</sub> evapd. in vacuo, and the residue treated with alkali gave 3.4 g. V, m. 147-7.5.degree. (MeOH). V (3 g.) was converted to 1.75 g. 3-bromoisoquinoline (VI), m. 63-4.degree. (aq. MeOH). 3-Chloroisoquinoline (8.8 g.), 100 cc. concd. NH<sub>4</sub>OH, and 1 g. CuSO<sub>4</sub> heated 30 hrs. at 140.degree. in an autoclave, made strongly basic, and extd. with CHCl<sub>3</sub> gave 5.3 g. Ia, m. 176-7.degree. (C<sub>6</sub>H<sub>6</sub>), similarly prepd. from VI. Ib m. 108-9.5.degree. (C<sub>6</sub>H<sub>6</sub>-cyclohexane). 5-Nitroisoquinoline (20 g.), 500 cc. MeOH, and 2 g. 5% Pd-C hydrogenated 2 hrs., evapd., and the residue crystd. from CHCl<sub>3</sub>-petr. ether gave 93% Ic, m. 129.5-30.5.degree. (C<sub>6</sub>H<sub>6</sub>-cyclohexane). m-MeOC<sub>6</sub>H<sub>4</sub>CHO (35.5 g.), 18 g. MeNO<sub>2</sub>, 125 cc. HOAc, and 12.5 g. NH<sub>4</sub>OAc refluxed 2 hrs. and poured into H<sub>2</sub>O gave 27 g. m-MeOC<sub>6</sub>H<sub>4</sub>CH:CHNO<sub>2</sub>, m. 91-2.degree. (C<sub>6</sub>H<sub>6</sub>), which was not reduced satisfactorily. 1,2,3,4-Tetrahydro-6-methoxyisoquinoline (2.42 g.) and 0.8 g. 30% Pd-C heated 0.25 hr. at 180-90.degree. in a stream of N, extd. with Et<sub>2</sub>O, the 2.1 g. oily product treated with 3 g. picric acid in 10 cc. Me<sub>2</sub>CO, the 2.9 g. picrate decompd. with aq. LiOH, extd. with Et<sub>2</sub>O, the 1.03 g. product refluxed 2 hrs. with 25 cc. concd. HBr, evapd. in vacuo, dissolved in 10 cc. H<sub>2</sub>O, and treated with aq. Na<sub>2</sub>CO<sub>3</sub> gave 0.85 g. 6-hydroxyisoquinoline (VII), m. 220.degree. (decompn.); dehydrogenation with Raney Ni in naphthalene was unsuccessful. Id, m. 211-12.degree. (C<sub>6</sub>H<sub>6</sub>), was prepd. from VII. 1,3-Dihydroxy-7-nitroisoquinoline (VIII) (52 g.), m. 291.degree. (decompn.), was prepd. from 56 g. 4-nitrohomophthalic acid in  $\alpha$ -C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>. VIII (2 g.) and 20 cc. POCl<sub>3</sub> heated 4 hrs. on the steam bath, decompd. with ice, and brought to pH 10 gave 1.18 g. 1,3-dichloro-7-nitroisoquinoline, m. 185.degree. (decompn.) (HOAc), but the reaction was not reproducible. 7-Hydroxyisoquinoline (1.25 g.), 4 cc. NH<sub>4</sub>SO<sub>3</sub> (concd. NH<sub>4</sub>OH satd. with SO<sub>2</sub>), and 20 cc. concd. NH<sub>4</sub>OH 16 hrs. at 140-50.degree. gave 1.1 g. Ie, m. 203-5.degree. (C<sub>6</sub>H<sub>6</sub>) after sublimation at 150.degree./0.3 mm. Ic (4.8 g.) in 12 cc. concd. HBr and 13 cc. H<sub>2</sub>O diazotized at 0.degree. with 2.3 g. NaNO<sub>2</sub> in 15 cc. H<sub>2</sub>O, added to 5.8 g. CuBr in 48 cc. HBr at 75.degree., and let stand 24 hrs. gave 5.1 g.

5-bromoisoquinoline (IX), m. 82-4.degree. (petr. ether). KNO<sub>3</sub> (2.4 g.) in 20 cc. concd. H<sub>2</sub>SO<sub>4</sub> added during 5 min. to 4.15 g. IX in 24 cc. concd. H<sub>2</sub>SO<sub>4</sub>, the mixt. let stand 1 hr. at room temp., poured on ice, and made alk. with NH<sub>4</sub>OH gave 5.05 g. 5-bromo-8-nitroisoquinoline (X), m. 139-41.degree. (MeOH). 5-Chloro-8-nitroisoquinoline (2 g.) and 12 g. NH<sub>4</sub>OAc added to 2 g. 6% Pd-CaCO<sub>3</sub> in abs. MeOH (previously shaken with H), hydrogenated 1 hr., the filtered soln. acidified with concd. HCl, the MeOH evapd. in vacuo, the residue in H<sub>2</sub>O made alk. with satd. Na<sub>2</sub>CO<sub>3</sub>, and extd. with CHCl<sub>3</sub> gave 1.02 g. If, m. 171-2.degree. (EtOAc); use of NaOAc in the reduction gave lower yields of If while reduction with Pd-C in MeOH in the presence of NaOAc gave 8-amino-5-chloroisoquinoline, from which the Cl was not removed on Raney Ni hydrogenation in alk. soln.; hydrogenation of X in MeOH over Pd-CaCO<sub>3</sub> gave colored intermediate products, while reduction of X in the presence of KOH gave a small yield of If. 2-Chloroquinazoline (0.5 g.) added slowly to 0.4 g. KOH in 5 g. PhOH, the mixt. heated 3 hrs. at 70.degree., and made alk. gave 0.58 g. 2-phenoxyquinazoline (XI), m. 124-6.degree. (petr. ether). XI (0.5 g.) and 5 g. NH<sub>4</sub>OAc heated 2 hrs. at 170-80.degree. and treated with H<sub>2</sub>O and 2N NaOH gave 0.35 g. IIIa, m. 200.degree. (EtOH). IIIb m. 271-2.degree. (EtOH). 6,2-O<sub>2</sub>N(H<sub>2</sub>N)C<sub>6</sub>H<sub>3</sub>CO<sub>2</sub>H (14.84 g.) and 29.4 cc. HCONH<sub>2</sub> 4.5 hrs. at 155-60.degree. gave 12.2 g. 4-hydroxy-5-nitroquinazoline (XII), m. 252-6.degree. (H<sub>2</sub>O). XII (7 g.) and POCl<sub>3</sub> gave 5.17 g. 4-chloro-5-nitroquinazoline (XIII), m. 142.degree. after sublimation at 140.degree./0.5 mm. Resublimed XIII (1 g.) in 150 cc. dry MeOCH<sub>2</sub>CH<sub>2</sub>OH and 0.5 g. 6% Pd-CaCO<sub>3</sub> hydrogenated 0.5 hr., evapd., oxidized with K<sub>3</sub>Fe(CN)<sub>6</sub>, and the product chromatographed gave 0.265 g. IIIc, m. 195-6.5.degree. (C<sub>6</sub>H<sub>6</sub>) after sublimation at 160.degree./1 mm. IIId, m. 213-14.degree. (C<sub>6</sub>H<sub>6</sub>), IIIe, m. 190-1.degree. (C<sub>6</sub>H<sub>6</sub>) after sublimation at 160.degree./0.5 mm., and IIIf, m. 150-1.degree. after sublimation at 120.degree./0.5 mm., were prepd. similarly by reduction at atm. pressure with 6% Pd-C. 1-Chloro-7-methoxyphthalazine (XIV) (7.4 g.), m. 142.degree. (decompn.), was obtained by refluxing 8.8 g. 1-OH compd. 0.5 hr. with 40 cc. POCl<sub>3</sub>. XIV (0.5 g.), 0.2 g. red P, and 5 cc. HI refluxed 1 hr., dild. with 5 cc. H<sub>2</sub>O, evapd. in vacuo, and the residue in 5 cc. H<sub>2</sub>O adjusted to pH 7 with NH<sub>4</sub>OH gave 0.3 g. 6-hydroxyphthalazine-0.5H<sub>2</sub>O, m. 300.degree. (decompn.) (H<sub>2</sub>O), which was not converted successfully to the 6-NH<sub>2</sub> compd. XIV refluxed with HBr gave 4,6-dihydroxyphthalazine, m. 310.degree. (decompn.) (H<sub>2</sub>O). 3,2-H<sub>2</sub>NC<sub>10</sub>H<sub>6</sub>CO<sub>2</sub>H (10 g.) was converted to 8.5 g. 4-hydroxy-6,7-benzoquinazoline (XV), m. 278.degree. (H<sub>2</sub>O). XV (1.3 g.) and 20 cc. POCl<sub>3</sub> refluxed 2 hrs. gave 0.98 g. 4-chloro-6,7-benzoquinazoline (XVI), m. 176-8.degree. after sublimation at 160.degree./0.1 mm. XVI (0.4 g.) in 50 cc. MeOCH<sub>2</sub>CH<sub>2</sub>OH hydrogenated 1.5 hrs. over 0.5 g. 8% Pd-CaCO<sub>3</sub> and the product in H<sub>2</sub>O oxidized with 1.4 g. K<sub>3</sub>Fe(CN)<sub>6</sub> gave 0.19 g. IV, m. 163-5.degree. (cyclohexane) after sublimation. XVI (0.23 g.) and 25 cc. satd. NH<sub>3</sub>-MeOH refluxed 2 hrs. gave 4-amino-6,7-benzoquinazoline, m. 365.degree. (decompn.) (EtOH) after repeated sublimation. XVI (2.1 g.) in 100 cc. warm C<sub>6</sub>H<sub>6</sub> added to 2 equivs. NaCH(CO<sub>2</sub>Et)<sub>2</sub> in 100 cc. C<sub>6</sub>H<sub>6</sub>, refluxed 3 hrs., let stand overnight, poured into H<sub>2</sub>O, the org. layer evapd., and the residue crystd. from EtOH gave 2.29 g. di-Et 6,7-benzoquinazol-4-ylmalonate (XVII), m. 172-5.degree.. XVII (1.5 g.), 0.6 g. KOH, and 60 cc. MeOH refluxed 3 hrs. gave 0.58 g. 6,7-benzoquinazol-4-ylacetate, m. 207-9.degree. (MeOH), hydrolyzed with boiling aq. NaOH to traces of 4-methyl-6,7-benzoquinazoline-1.5H<sub>2</sub>O, m. 124-6.degree. (petr. ether). I (5 g.), 10 cc. MeI, and MeOH refluxed 2 hrs. gave I methiodide, m. 160-1.5.degree. (EtOH), which was shaken with 50 cc. H<sub>2</sub>O and excess freshly pptd. AgCl for 12 hrs., filtered, the filtrate evapd., and I methochloride crystd. under anhyd. conditions from EtOH-Et<sub>2</sub>O. Quinoline methochloride, the very deliquescent II

methochloride-0.5H<sub>2</sub>O, and 4-methylcinnoline methochloride-H<sub>2</sub>O were prepd. similarly.

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NEWS 7 Sep 03 JAPIO has been reloaded and enhanced  
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NEWS 9 Sep 16 CA Section Thesaurus available in CAPLUS and CA  
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DICTIONARY FILE UPDATES:   2 MAY 2003    HIGHEST RN 509953-09-7

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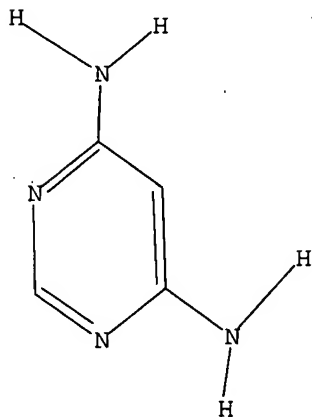
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L1 HAS NO ANSWERS

L1 STR



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=> s l1

SAMPLE SEARCH INITIATED 10:52:23 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 630 TO ITERATE

100.0% PROCESSED 630 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 11095 TO 14105

PROJECTED ANSWERS: 1384 TO 2576

L2 50 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 10:52:31 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 12545 TO ITERATE

100.0% PROCESSED 12545 ITERATIONS

1870 ANSWERS

SEARCH TIME: 00.00.01

L3 1870 SEA SSS FUL L1

=&gt; file caplus

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148.36

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FILE COVERS 1907 - 3 May 2003 VOL 138 ISS 19

FILE LAST UPDATED: 2 May 2003 (20030502/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=&gt; s l3

L4 1498 L3

=&gt; s l4 and quinoxaline

L5 10 L4 AND QUINOXALINE

=&gt; d l5 fbib hitstr abs total

L5 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 2002:224567 CAPLUS

DN 137:109252

TI On condensation reactions of aceanthrenequinone: novel heterocycles

AU Amer, Atef M.; El-Mobayed, Medhat; Ateya, Abdel M.; Muhdi, Tarek S.

CS Chemistry Department, Faculty of Science, Zagazig University, Zagazig, Egypt

SO Monatshefte fuer Chemie (2002), 133(1), 79-88

CODEN: MOCMB7; ISSN: 0026-9247

PB Springer-Verlag Wien

DT Journal

LA English

OS CASREACT 137:109252

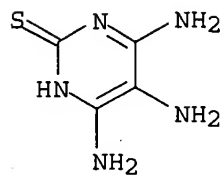
IT 1073-99-0, 4,5,6-Triamino-2-pyrimidinethiol 22715-34-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(heterocycle prepn. by condensation reactions of aceanthrenequinone)

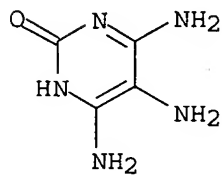
RN 1073-99-0 CAPLUS

CN 2(1H)-Pyrimidinethione, 4,5,6-triamino- (9CI) (CA INDEX NAME)

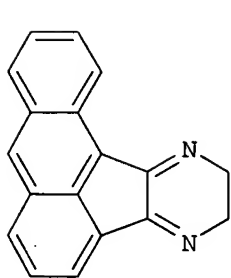


RN 22715-34-0 CAPLUS

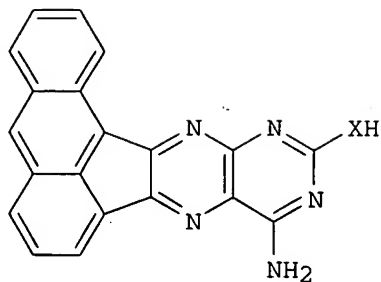
CN 2(1H)-Pyrimidinone, 4,5,6-triamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



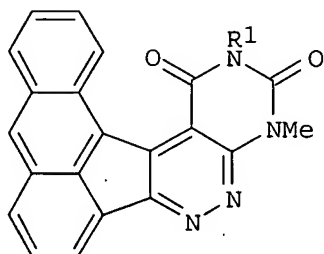
GI



I



II



III

AB It was found that aceanthrenequinone can be condensed with ethylenediamine, 1,2-diaminobenzene, 4-nitro-1,2-diaminobenzene, 1,2-diaminoanthrenequinone, and 4,5,6-triaminopyrimidine derivs. to give aceanthryleno[1,2-b]pyrazine (I) and aceanthryleno[1,2-g]pteridine derivs. (II; X = O, S). Condensation of aceanthrenequinone with 2-aminoguanidine, semicarbazide, and thiosemicarbazide yielded aceanthryleno[1,2-e]triazines; condensation with 6-hydrazinopyrimidine derivs. gave 3,4-aceanthrylenopyrimido[4,5-c]pyridazines (III; R1 = Me, H). Reaction

of aceanthrenequinone with 2-cyanoethanoic acid hydrazide afforded 10,11-dihydro-10-oxoaceanthryleno[1,2-c]pyridazine-9-carbonitrile. Treatment of aceanthrenequinone with malononitrile and hydrazine hydrate resulted in 10-aminoaceanthryleno[1,2-c]pyridazine-9-carbonitrile. The antibacterial effects of the prepd. compds. were tested. Three of the compds. were tested against 60 cancer types.

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 2001:923229 CAPLUS

DN 136:58496

TI Hair dyeing compositions containing **quinoxaline** derivatives

IN Gross, Wibke; Hoeffkes, Horst; Martin, Hans-Dieter; Moeller, Hinrich; Oberkobusch, Doris

PA Henkel K.-G.a.A., Germany

SO Ger. Offen., 22 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

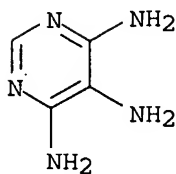
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10029929	A1	20011220	DE 2000-10029929	20000617
	WO 2001097754	A2	20011227	WO 2001-EP6544	20010609
	WO 2001097754	A3	20020523		
	W: AU, JP, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	EP 1292271	A2	20030319	DE 2000-10029929A	20000617
				EP 2001-957836	20010609
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
				DE 2000-10029929A	20000617
				WO 2001-EP6544 W	20010609

OS MARPAT 136:58496

IT **118-70-7**, 4,5,6-Triaminopyrimidine **1004-74-6**,  
2,4,5,6-Tetraaminopyrimidine **5392-28-9** **22715-34-0**,  
2-Hydroxy-4,5,6-Triaminopyrimidine **62496-02-0**,  
2-Methylamino-4,5,6-triaminopyrimidine  
RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
(hair dyeing compns. contg. **quinoxaline** derivs.)

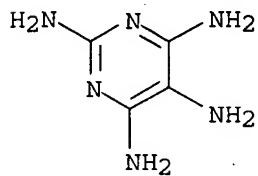
RN 118-70-7 CAPLUS

CN 4,5,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



RN 1004-74-6 CAPLUS

CN Pyrimidinetetramine (9CI) (CA INDEX NAME)

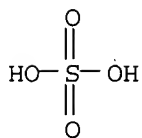


RN 5392-28-9 CAPLUS  
CN Pyrimidinetetramine, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 7664-93-9

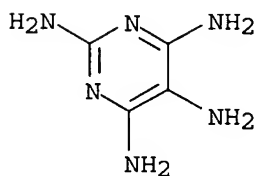
CMF H2 O4 S



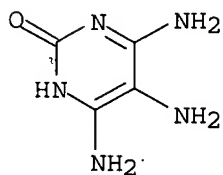
CM 2

CRN 1004-74-6

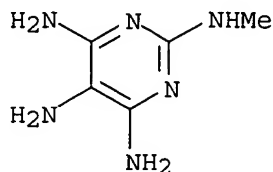
CMF C4 H8 N6



RN 22715-34-0 CAPLUS  
CN 2(1H)-Pyrimidinone, 4,5,6-triamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 62496-02-0 CAPLUS  
CN Pyrimidinetetramine, N2-methyl- (9CI) (CA INDEX NAME)



AB Hair dye compns. contain at least one **quinoxaline** deriv. contg. e.g., C1-4 alkenyl, hydroxyalkyl, carboxyalkyl groups, and halo groups. Thus, 1,1,3-trimethylcyclo-2-penten[1,2-b]quinoxaline-2-carboxaldehyde (I) was prepd. in a series of steps and formulated into a hair dye formulation contg. I 4.4, Natrosol 250HR 2.0 and water to 100.0 g.

L5 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 2001:45037 CAPLUS

DN 134:120569

TI Hair dyeing preparations containing heterocyclic aldehydes or ketones

IN Moeller, Hinrich; Oberkobusch, Doris; Hoeffkes, Horst

PA Henkel K.-G.a.a., Germany

SO Ger. Offen., 12 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19933187	A1	20010118	DE 1999-19933187	19990715
	WO 2001005359	A2	20010125	WO 2000-EP6399	20000706
	WO 2001005359	A3	20010426		
	W: AU, JP, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				

DE 1999-19933187A 19990715

OS MARPAT 134:120569

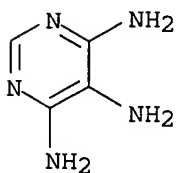
IT **118-70-7**, 4,5,6-Triaminopyrimidine **1004-74-6**,  
2,4,5,6-Tetraaminopyrimidine **22715-34-0**, 2-Hydroxy-4,5,6-  
triaminopyrimidine **62496-02-0**, 2-Methylamino-4,5,6-  
triaminopyrimidine

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES  
(Uses)

(hair dyeing preps. contg. heterocyclic aldehydes or ketones)

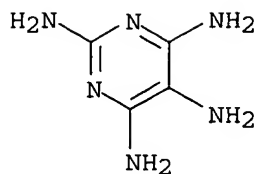
RN 118-70-7 CAPLUS

CN 4,5,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



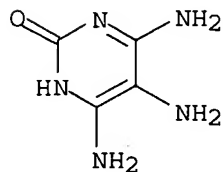
RN 1004-74-6 CAPLUS

CN Pyrimidinetetramine (9CI) (CA INDEX NAME)



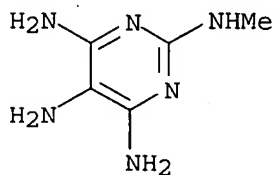
RN 22715-34-0 CAPLUS

CN 2(1H)-Pyrimidinone, 4,5,6-triamino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

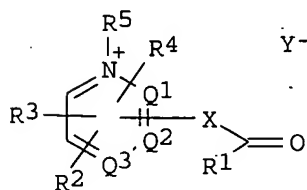


RN 62496-02-0 CAPLUS

CN Pyrimidinetetramine, N2-methyl- (9CI) (CA INDEX NAME)



GI



AB The invention concerns compns. for dyeing keratin fibers, esp. hair, that contain at least one heterocyclic aldehyde or ketone of the formula (I) and a compd. from the group of arom. amines, hydroxyls, including heterocycles, and compds. with active CH groups. In I R1 = H, C1-C4 alkyl, aryl, heteroaryl; R2, R3, R4 = H, C1-C4 alkyl, hydroxyalkyl, carboxyalkyl, sulfoalkyl, aryl, aralkyl, heteroaryl; Q1, Q2, Q3 = combination of two C and one N, the N can be quaternized; X = vinylene or vinylene deriv.; Y = halide, benzene sulfonate, p-toluene sulfonate, methane sulfonate, tetrachlorozincate, nitrogen oxide, oxide. Thus 2-formyl-1-methylquinoxalinium-trifluoromethanesulfonate was synthesized from **quinoxaline**-2-carboxaldehyde and trifluoromethanesulfonic acid Me ester. The product was used in hair dyeing compns.; depending on the selected other dye(s), different colors were obtained; e.g the

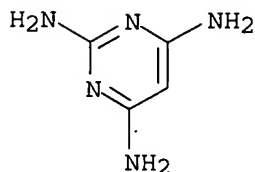
combination with 2-methyl-3-amino-6-methoxypyridine dihydrochloride resulted redish brown hair color.

L5 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2003 ACS  
 AN 1996:333008 CAPLUS  
 DN 125:127644  
 TI Method for obtaining improved image contrast in migration imaging members  
 IN Limburg, William W.; Mammino, Joseph; Liebermann, George; Griffiths, Clifford H.; Shahin, Michael M.; Malhotra, Shadi L.; Chen, Liqin; Perron, Marie-Eve  
 PA Xerox Corp., USA  
 SO U.S., 147 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1

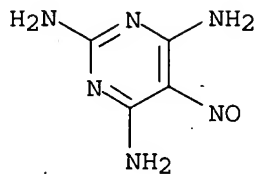
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PI	US 5514505	A	19960507	US 1995-441360	19950515
	CA 2169980	AA	19961116	CA 1996-2169980	19960221
	CA 2169980	C	20010424		
				US 1995-441360 A	19950515
	JP 08314240	A2	19961129	JP 1996-113456	19960508
				US 1995-441360 A	19950515
	EP 743573	A2	19961120	EP 1996-303359	19960514
	EP 743573	A3	19970305		
	EP 743573	B1	20000906		
	R: DE, FR, GB				

US 1995-441360 A 19950515

OS MARPAT 125:127644  
 IT **1004-38-2**, 2,4,6-Triaminopyrimidine **1006-23-1**,  
 5-Nitroso-2,4,6-triaminopyrimidine **49647-58-7**,  
 2,4,5,6-Tetraaminopyrimidine sulfate **49721-45-1**  
**116295-66-0 120407-07-0**  
 RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)  
 (transparentizing agent for electrophotog. migration imaging members)  
 RN 1004-38-2 CAPLUS  
 CN 2,4,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



RN 1006-23-1 CAPLUS  
 CN 2,4,6-Pyrimidinetriamine, 5-nitroso- (9CI) (CA INDEX NAME)



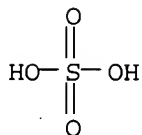
RN 49647-58-7 CAPLUS

CN Pyrimidinetetramine, sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 7664-93-9

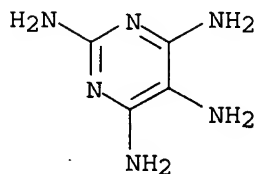
CMF H2 O4 S



CM 2

CRN 1004-74-6

CMF C4 H8 N6



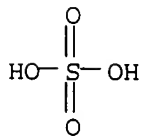
RN 49721-45-1 CAPLUS

CN 4,5,6-Pyrimidinetriamine, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

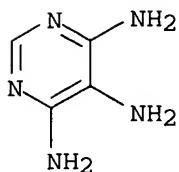
CRN 7664-93-9

CMF H2 O4 S



CM 2

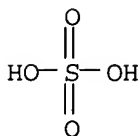
CRN 118-70-7  
CMF C4 H7 N5



RN 116295-66-0 CAPLUS  
CN 2(1H)-Pyrimidinethione, 4,5,6-triamino-, sulfate (1:1) (9CI) (CA INDEX NAME)

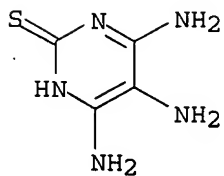
CM 1

CRN 7664-93-9  
CMF H2 O4 S

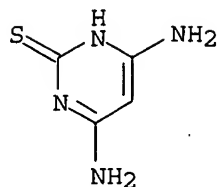


CM 2

CRN 1073-99-0  
CMF C4 H7 N5 S



RN 120407-07-0 CAPLUS  
CN 2(1H)-Pyrimidinethione, 4,6-diamino-, hydrate (2:1) (9CI) (CA INDEX NAME)



1/2 H<sub>2</sub>O

AB Disclosed is a process which comprises (a) providing a migration imaging member comprising (1) a substrate and (2) a softenable layer comprising a softenable material and a photosensitive migration marking material present in the softenable layer as a monolayer of particles situated at or near the surface of the softenable layer spaced from the substrate, (b) uniformly charging the imaging member, (c) imagewise exposing the charged imaging member to activating radiation at a wavelength to which the migration marking material is sensitive, (d) causing the softenable material to soften and enabling a first portion of the migration marking material to migrate through the softenable material toward the substrate in an imagewise pattern while a second portion of the migration marking material remains substantially unmigrated within the softenable layer, and (e) contacting the second portion of the migration marking material with a transparentizing agent which transparentizes the migration marking material.

L5 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 1984:571208 CAPLUS

DN 101:171208

TI 1-Halo-1-(acylamino)-2-alkanones as synthons for the preparation of **quinoxalines** and pteridines

AU Zav'yalov, S. I.; Ezhova, G. I.; Budkova, T. K.

CS Inst. Org. Khim. im. Zelinskogo, Moscow, USSR

SO Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1984), (7), 1590-3  
CODEN: IASKA6; ISSN: 0002-3353

DT Journal

LA Russian

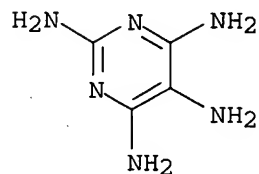
OS CASREACT 101:171208

IT **1004-74-6**

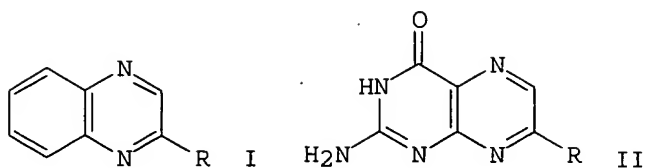
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation of, with (acylamino)haloalkanones)

RN 1004-74-6 CAPLUS

CN Pyrimidinetetramine (9CI) (CA INDEX NAME)



GI



AB Alkylquinoxalines I (R = Me, Et, Pr) and 7-alkylpteridines II (R = Me, Et) were prepd. in 52-70% and 68-80% yields, resp., by cyclocondensation of RCOCHXNHCOR<sub>1</sub> (X = Cl, Br; R<sub>1</sub> = Me, Ph) with o-phenylenediamine or 2,5,6-triamino-2(1H)-pyrimidinone (III). Treating AcNHCHBrCOMe with N<sub>2</sub>H<sub>4</sub>.cntdot.H<sub>2</sub>O gave 29% HC(:NHNH<sub>2</sub>)C(:NHNH<sub>2</sub>)Me which was cyclocondensed with III to give 84% 6-methylpteridine and 16% II (R = Me).

L5 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 1981:208808 CAPLUS

DN 94:208808

TI Studies in the heterocyclic series. XVIII. Utilization of 4-aminopyrimidine chemistry in 1,4,7,9-tetraazabenzob[thiazine synthesis

AU Okafor, Charles O.

CS Dep. Chem., Univ. Nigeria, Nigeria, Nigeria

SO Journal of Heterocyclic Chemistry (1980), 17(7), 1587-92

CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

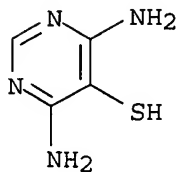
LA English

IT 77709-01-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and cyclization with dichlorophenoxalines)

RN 77709-01-4 CAPLUS

CN 5-Pyrimidinethiol, 4,6-diamino- (9CI) (CA INDEX NAME)

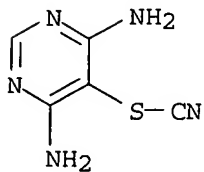


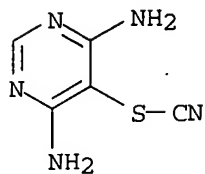
IT 30161-88-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and hydrolysis of)

RN 30161-88-7 CAPLUS

CN Thiocyanic acid, 4,6-diamino-5-pyrimidinyl ester (9CI) (CA INDEX NAME)





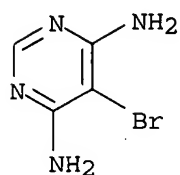
IT 58023-98-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(prepn. and reaction with thiocyanate)

RN 58023-98-6 CAPLUS

CN 4,6-Pyrimidinediamine, 5-bromo- (9CI) (CA INDEX NAME)



IT 77709-02-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with sodium thiocyanate)

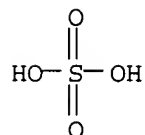
RN 77709-02-5 CAPLUS

CN 4,6-Pyrimidinediamine, sulfate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 7664-93-9

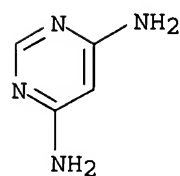
CMF H2 O4 S



CM 2

CRN 2434-56-2

CMF C4 H6 N4



Welcome to STN International! Enter x:x

LOGINID:sssptal611sxp

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 2 Apr 08 "Ask CAS" for self-help around the clock  
NEWS 3 Jun 03 New e-mail delivery for search results now available  
NEWS 4 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN  
NEWS 5 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)  
now available on STN  
NEWS 6 Aug 26 Sequence searching in REGISTRY enhanced  
NEWS 7 Sep 03 JAPIO has been reloaded and enhanced  
NEWS 8 Sep 16 Experimental properties added to the REGISTRY file  
NEWS 9 Sep 16 CA Section Thesaurus available in CAPLUS and CA  
NEWS 10 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985  
NEWS 11 Oct 24 BEILSTEIN adds new search fields  
NEWS 12 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN  
NEWS 13 Nov 18 DKILIT has been renamed APOLLIT  
NEWS 14 Nov 25 More calculated properties added to REGISTRY  
NEWS 15 Dec 04 CSA files on STN  
NEWS 16 Dec 17 PCTFULL now covers WP/PCT Applications from 1978 to date  
NEWS 17 Dec 17 TOXCENTER enhanced with additional content  
NEWS 18 Dec 17 Adis Clinical Trials Insight now available on STN  
NEWS 19 Jan 29 Simultaneous left and right truncation added to COMPENDEX,  
ENERGY, INSPEC  
NEWS 20 Feb 13 CANCERLIT is no longer being updated  
NEWS 21 Feb 24 METADEX enhancements  
NEWS 22 Feb 24 PCTGEN now available on STN  
NEWS 23 Feb 24 TEMA now available on STN  
NEWS 24 Feb 26 NTIS now allows simultaneous left and right truncation  
NEWS 25 Feb 26 PCTFULL now contains images  
NEWS 26 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results  
NEWS 27 Mar 19 APOLLIT offering free connect time in April 2003  
NEWS 28 Mar 20 EVENTLINE will be removed from STN  
NEWS 29 Mar 24 PATDPAFULL now available on STN  
NEWS 30 Mar 24 Additional information for trade-named substances without  
structures available in REGISTRY  
NEWS 31 Apr 11 Display formats in DGENE enhanced  
NEWS 32 Apr 14 MEDLINE Reload  
NEWS 33 Apr 17 Polymer searching in REGISTRY enhanced  
NEWS 34 Apr 21 Indexing from 1947 to 1956 being added to records in CA/CAPLUS  
NEWS 35 Apr 21 New current-awareness alert (SDI) frequency in  
WPIDS/WPINDEX/WPIX  
NEWS 36 Apr 28 RDISCLOSURE now available on STN  
  
NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT  
MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),  
AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003  
NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS INTER      General Internet Information  
NEWS LOGIN      Welcome Banner and News Items  
NEWS PHONE      Direct Dial and Telecommunication Network Access to STN  
NEWS WWW        CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 11:00:30 ON 03 MAY 2003

=> le reg

LE IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.  
For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 11:00:45 ON 03 MAY 2003

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STRUCTURE FILE UPDATES:      2 MAY 2003    HIGHEST RN 509953-09-7

DICTIONARY FILE UPDATES:    2 MAY 2003    HIGHEST RN 509953-09-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when

conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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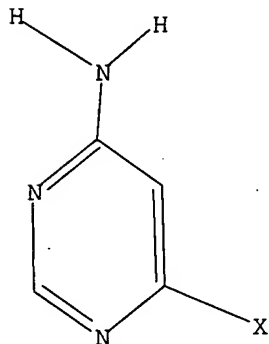
Uploading 10077150.5

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:01:00 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 512 TO ITERATE

100.0% PROCESSED 512 ITERATIONS

38 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 8883 TO 11597

PROJECTED ANSWERS: 391 TO 1129

L2 38 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 11:01:07 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 10484 TO ITERATE

100.0% PROCESSED 10484 ITERATIONS

762 ANSWERS

SEARCH TIME: 00.00.01

L3 762 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
148.15	148.36

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 11:01:13 ON 03 MAY 2003  
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FILE COVERS 1907 - 3 May 2003 VOL 138 ISS 19  
FILE LAST UPDATED: 2 May 2003 (20030502/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 742 L3

=> s l4 and qunopxaline

L5 0 L4 AND QUNOPXALINE

=> s l4 and quinoxaline

L6 2 L4 AND QUINOXALINE

=> d l6 fbib hitstr abs total

L6 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS

AN 1996:333008 CAPLUS

DN 125:127644

TI Method for obtaining improved image contrast in migration imaging members  
IN Limburg, William W.; Mammino, Joseph; Liebermann, George; Griffiths, Clifford H.; Shahin, Michael M.; Malhotra, Shadi L.; Chen, Liqin; Perron, Marie-Eve

PA Xerox Corp., USA

SO U.S., 147 pp.

CODEN: USXXAM

DT Patent

LA English

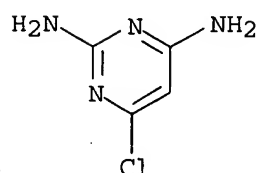
FAN.CNT 1

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	CA 2169980	C	20010424		
				US 1995-441360 A	19950515

JP 08314240 A2 19961129 JP 1996-113456 19960508  
US 1995-441360 A 19950515  
EP 743573 A2 19961120 EP 1996-303359 19960514  
EP 743573 A3 19970305  
EP 743573 B1 20000906  
R: DE, FR, GB

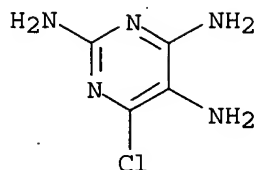
US 1995-441360 A 19950515

OS MARPAT 125:127644  
IT 156-83-2, 2,6-Diamino-4-chloropyrimidine  
RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)  
(transparentizing agent for electrophotog. migration imaging members)  
RN 156-83-2 CAPLUS  
CN 2,4-Pyrimidinediamine, 6-chloro- (9CI) (CA INDEX NAME)



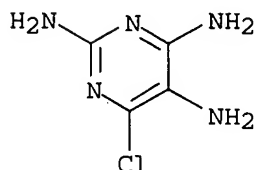
AB Disclosed is a process which comprises (a) providing a migration imaging member comprising (1) a substrate and (2) a softenable layer comprising a softenable material and a photosensitive migration marking material present in the softenable layer as a monolayer of particles situated at or near the surface of the softenable layer spaced from the substrate, (b) uniformly charging the imaging member, (c) imagewise exposing the charged imaging member to activating radiation at a wavelength to which the migration marking material is sensitive, (d) causing the softenable material to soften and enabling a first portion of the migration marking material to migrate through the softenable material toward the substrate in an imagewise pattern while a second portion of the migration marking material remains substantially unmigrated within the softenable layer, and (e) contacting the second portion of the migration marking material with a transparentizing agent which transparentizes the migration marking material.

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS  
AN 1963:33381 CAPLUS  
DN 58:33381  
OREF 58:5675f-h,5676a-b  
TI v-Triazolo[4,5-d]pyrimidines. II. O-Substituted derivatives of 8-azaguanine and 8-azahypoxanthine  
AU Fulmer Shealy, Y.; Clayton, Joe D.; Allen O'Dell, C.; Montgomery, John A.  
CS Southern Res. Inst., Birmingham, AL  
SO J. Org. Chem. (1962), 27, 4518-23  
CODEN: JOCEAH; ISSN: 0022-3263  
DT Journal  
LA Unavailable  
IT 1194-78-1, Pyrimidine, 2,4,5-triamino-6-chloro- 89303-96-8  
, Pyrimidine, 2,4,5-triamino-6-chloro-, hydrochloride  
(prepn. of)  
RN 1194-78-1 CAPLUS  
CN 2,4,5-Pyrimidinetriamine, 6-chloro- (9CI) (CA INDEX NAME)



RN 89303-96-8 CAPLUS

CN Pyrimidine, 2,4,5-triamino-6-chloro-, hydrochloride (7CI) (CA INDEX NAME)

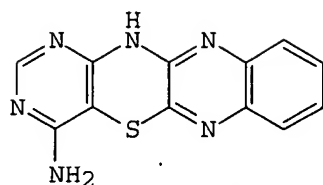


●x HCl

GI For diagram(s), see printed CA Issue.

AB cf. CA 56, 14277g. 5-Amino-7-chloro-v-triazolo[4,5-d]pyrimidine (I) was prepd. from 2,4,5-triamino-6-chloropyrimidine and isoamyl nitrite. 7-Chloro-v-triazolo[4,5-d]pyrimidine was obtained in dioxane soln. by the same method. These compds., useful intermediates for the preparation of a variety of 7-substituted v-triazolo[4,5-d]pyrimidines, were employed in the synthesis of 7-alkoxy- and 7-aryloxy-v-triazolo-[4,5-d] pyrimidines. Preparation and some reactions of 3-bromo-4,5-diaminopyridine. Jan Sylwester Wieczorek and Tadeusz Talik (Politechnika, Wroclaw, Poland). Roczniki Chem. 36, 967-70(1962). I (R = Br, R1 = NH2, R2 = R3 = H) (15 g.) in 75 ml. concd. H2SO4 treated with 30 ml. concd. HNO3 (d. 1.52) at 0 to -10.degree. gave 84.6% I (R = Br, R1 = NHNO2, R2 = R3 = H) (II), m. 203.degree. (decompn.). II (15 g.), when heated with 90 ml. H2SO4 on a steam bath, poured into 500 g. ice and alkalized, gave 14.6 g. I (R = Br, R1 = NH2, R2 = NO2, R3 = H) (III), m. 179-80.degree.. III (3 g.) in 90 ml. glacial AcOH was reduced with 9 g. powd. Fe, heated 1 hr. on steam bath, excess AcOH evapd. under reduced pressure, the residue alkalized, and extd. continuously with Et2O to give 1.8 g. I (R = Br, R1 = R2 = NH2, R3 = H) (IV), m. 140-1.degree.; picrate m. 220-1.degree.. Redn. of III with SnCl2 gave C5H5N3ClBr (m. 206-8.degree., 63.6%), probably I (R = Br, R1 = R2 = NH2, R3 = Cl). IV reacted with phenanthrenequinone to yield 9,10-phenanthro-5,6-(3-bromo-4,5-pyrido)pyrazine, m. 224-6.degree., with 100% HCO2H, 4,5-(3-bromo-4,5-pyrido)imidazole, m. 292-4.degree., and with Bz2, V, m. 198-200.degree..

GI



I

AB Tetraazabenzophenothiazine derivs., e.g. I, were prepd. from 4-aminopyrimidines. This new heterocyclic ring was obtained by converting a 4-aminopyrimidine to the corresponding 5-thiocyanato deriv. followed by hydrolysis and subsequent treatment with 2,3-dichloroquinoxaline. Several derivs. were obtained by using suitable substituted starting materials. Nitration with HNO<sub>3</sub>-H<sub>2</sub>SO<sub>4</sub> gave the corresponding 13-nitro derivs.

L5 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 1964:64994 CAPLUS

DN 60:64994

OREF 60:11441f-g

TI X-ray powder diffraction patterns of solid hydrocarbons, derivatives of hydrocarbons, phenols, and organic bases

AU Hofer, L. J. E.; Peebles, W. C.; Bean, E. H.

CS U.S. Bur. of Mines, Washington, DC

SO U.S., Bur. Mines, Bull. (1963), No. 613, 59 pp.

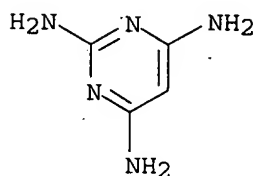
DT Journal

LA Unavailable

IT 1004-38-2, Pyrimidine, 2,4,6-triamino-  
(x-ray diffraction pattern for)

RN 1004-38-2 CAPLUS

CN 2,4,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



AB Included are compds. of interest in research involving fuels, coal tar dyes, plastics, pharmaceutical, agricultural chemicals, carcinogens, air pollutants, and other public health problems. X-ray powder diffraction patterns (178) are presented of aromatic hydrocarbons, 2,4,7-trinitro-9-fluorenone derivs. of aromatic hydrocarbons, phenols, and org. bases for pos. identification of solid org. compds.

L5 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 1962:21276 CAPLUS

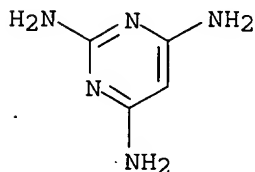
DN 56:21276

OREF 56:4039d-g

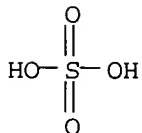
TI Screening of antineoplastic agents with *Neurospora crassa*

AU Fuerst, Robert

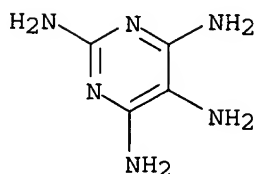
CS Texas Woman's Univ., Denton  
SO Develop. Ind. Microbiol. (1960), 1, 101-7  
DT Journal  
LA Unavailable  
IT 1004-38-2, Pyrimidine, 2,4,6-triamino- 49647-58-7,  
Pyrimidine, 2,4,5,6-tetraamino-, sulfate  
(effect on 4-aminopyrazolo[3,4-d]pyrimidine deriv. inhibition of  
Neurospora crassa)  
RN 1004-38-2 CAPLUS  
CN 2,4,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)



RN 49647-58-7 CAPLUS  
CN Pyrimidinetetramine, sulfate (9CI) (CA INDEX NAME)  
CM 1  
CRN 7664-93-9  
CMF H2 O4 S



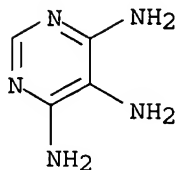
CM 2  
CRN 1004-74-6  
CMF C4 H8 N6



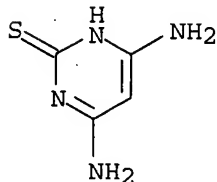
AB Compds. of the 4-aminopyrazolo[3,4-d]pyrimidine (4-APP) compds. and  
derivs. of 4-APP were tested as antineoplastic agents with *N. crassa* in  
liquid culture. Two recent derivs. of 4-APP, 1-methyl-4-  
octylaminopyrazolo[3,4-d]pyrimidine and 4-heptylamino-1-methylpyrazolo[3,4-  
d]pyrimidine were more inhibitory to *Neurospora* than 4-APP itself.  
**Quinoxalines** and isonitrosomalonitriles were also studied;  
2-amino-6-purinethiol and many of its derivs. gave little or no

inhibition. Of the most important inhibitors studied, 6-diazo-5-oxonorleucine (DON) gave the best inhibition in lowest doses. Testing DON by the Neurospora agar plate method gave results analogous to the liquid culture method. Thiophene compds. showed definite inhibition but inject/on into C57 black mice resulted in some paralysis and death; 4-(2-thienyl)butanoic acid was the best inhibitor; 2-heptylthiophene and 2-(2-methyl-propyl)thiophene also inhibited well. Aminopterin and 4-APP tested together resulted in 4-APP acting as a relief agent and did not reverse aminopterin inhibition. Inhibition by 4-APP was not affected by 6-methyl-2-thiouracil or purine. 2-Aminopurine and 2,4,5-triamino-6-hydroxypyrimidine sulfate increased 4-APP inhibition. DON with azaserine, 4-APP with azaserine, and DON with 8-azaadenine resulted in enhanced inhibition. 8-Azaadenine with azaserine did not affect inhibition. Neurospora as a tool for new chem. antineoplastic agents is important but not more important than the use of other microorganisms or tissue culture techniques or animal-tumor expts.

L5 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2003 ACS  
AN 1957:11927 CAPLUS  
DN 51:11927  
OREF 51:2455d-h  
TI Legal's color reaction  
AU Tanabe, Yoshihisa; Kamiya, Akiko  
CS Kanazawa Univ.  
SO Ann. Rept. Fac. Pharm., Kanazawa Univ. (1956), 6, 12-15  
DT Journal  
LA Unavailable  
IT 118-70-7, Pyrimidine, 4,5,6-triamino- 1004-39-3,  
2-Pyrimidinethiol, 4,6-diamino- 1073-99-0, 2-Pyrimidinethiol,  
4,5,6-triamino- 2434-56-2, Pyrimidine, 4,6-diamino-  
5122-36-1, Formamide, N-(4,6-diamino-5-pyrimidinyl)-  
(detection of)  
RN 118-70-7 CAPLUS  
CN 4,5,6-Pyrimidinetriamine (9CI) (CA INDEX NAME)

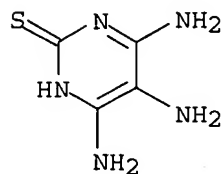


RN 1004-39-3 CAPLUS  
CN 2(1H)-Pyrimidinethione, 4,6-diamino- (7CI, 9CI) (CA INDEX NAME)



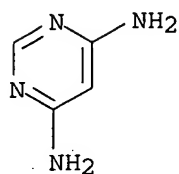
RN 1073-99-0 CAPLUS

CN 2(1H)-Pyrimidinethione, 4,5,6-triamino- (9CI) (CA INDEX NAME)



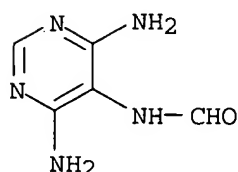
RN 2434-56-2 CAPLUS

CN 4,6-Pyrimidinediamine (9CI) (CA INDEX NAME)



RN 5122-36-1 CAPLUS

CN Formamide, N-(4,6-diamino-5-pyrimidinyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



AB Legal's color reaction was carried out with barbituric acid, purine, pyrimidine, imidazole, etc., and their derivs. The compd., color in basic medium, and color in acidic medium are given (\*signifies the color when warmed): barbituric acid, yellow, light yellow (bluish green\*); 5-nitrobarbituric acid, orange, light yellow (bluish green\*); 5-aminobarbituric acid, yellow, green; 5-isonitrosobarbituric acid, red, deep blue; 5-hydroxybarbituric acid, yellowish brown, orange to red; 5,5-diethylbarbituric acid, yellow, light yellow; 5-ethyl-5-phenylbarbituric acid, yellow, light yellow; 5-ethyl-5-isoamylbarbituric acid, yellow, light yellow; 5-ethyl-5-(1-methylbutyl)barbituric acid, yellow, light yellow; 1-methyl-5-ethyl-5-phenylbarbituric acid, yellow, light yellow; 1,5-dimethyl-5-cyclohexenylbarbituric acid, yellow, light yellow; 5-ethyl-5-cyclohexenylbarbituric acid, yellow, light yellow; thiobarbituric acid, yellow, dark green to dark blue; 5-nitrothiobarbituric acid, orange-yellow, light brown; 5-aminothiobarbituric acid, reddish brown, dark-bluish green; urea, yellow, light yellow; thiourea, yellow, blue to dark blue; methionine, yellow, reddish orange\*; theophylline, yellow, light yellow; theobromine, yellow, light yellow; xanthine, yellow, light yellow; caffeine, yellow, light yellow; uric acid, yellow, bluish green\*; 4,6-diaminopyrimidine-2-thiol, dark yellow, blue; 4,5,6-triaminopyrimidine-2-thiol, dark yellow, bluish green; 4,6-diaminopyrimidine, yellow, light yellow; 4,5,6-

triaminopyrimidine, yellow, light-reddish orange to reddish orange; 5-formylamino-4,6-diaminopyrimidine, yellow, light yellow; benzimidazole, yellowish green, crimson (limit 50 .gamma./cc.); naphthoimidazole, yellow, reddish orange (limit 100 .gamma./cc.); quinazoline, blood-red, blood-red; **quinoxaline**, blood-red, reddish violet; 1-(2-benzimidazolyl)1,2,3,4,5-pentahydroxypentane, yellow, light yellow; 1-(2-quinoxaliny)1,2,3,4-tetrahydroxybutane, yellow, light yellow; 2-methylbenzothiazole-EtI, bluish green, violet; 2-ethylbenzothiazole-EtI, yellow, reddish brown; quinaldine-EtI, green, bluish violet; lepidine-EtI, green, bluish violet; 2,4-dimethylthiazole-EtI, blood-red, violet; benzoxazole-EtI, yellow, light yellow; 2-adeninethiol, yellowish brown, green; adenine, yellow, reddish violet; guanine, yellow, white ppt.; 8-azaguanine, yellow, white ppt.

L5 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2003 ACS

AN 1952:54597 CAPLUS

DN 46:54597

OREF 46:9094h-i,9095a-h

TI Organic reactions in aqueous solution at room temperature. I. The influence of pH on condensations involving the linking of carbon to nitrogen and of carbon to carbon

AU Haley, C. A. C.; Maitland, P.

CS Univ. Cambridge, UK

SO J. Chem. Soc. (1951) 3155-74

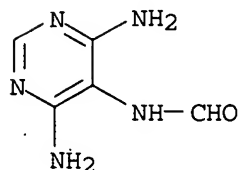
DT Journal

LA Unavailable

IT **5122-36-1**, Formamide, N-(4,6-diamino-5-pyrimidinyl)-(prepn. of)

RN 5122-36-1 CAPLUS

CN Formamide, N-(4,6-diamino-5-pyrimidinyl)- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



AB The object of this series of papers is to broaden the field initiated by Robinson and Schopf and usually termed "syntheses under physiol. (or cell-possible) conditions" in relation to both biochem. problems and general org. synthetical methods. Extensive (rather than intensive) investigations have shown that H<sub>2</sub>O at room temp. is an effective medium for some very simple condensations involving substances contg. the naturally occurring groups CHO, CO, NH<sub>2</sub>, CONH<sub>2</sub>, NH<sub>2</sub>C:NH, CH<sub>2</sub>CN, CH<sub>2</sub>CO, COCH<sub>2</sub>CO, COCH<sub>2</sub>CH<sub>2</sub>CO (and HCO<sub>2</sub>H), leading to well-known examples of Schiff bases, and **quinoxaline**, diazepine, pyrimidine, glyoxaline, pyrrole, and pyridine derivs. Some failures have suggested that in this type of work, a CH<sub>2</sub> group requires activation from both sides for successful condensation. In 2 cases of Claisen-Knoevenagel condensations, glycine is a useful catalyst. As found by Schopf in other cases, variation of the pH has striking effects on the yields. The reaction conditions differed from those used by Robinson and Schopf in that, whereas they usually had to isolate their products from soln., H. and M. chose H<sub>2</sub>O-sol. reactants which produced very difficultly sol. products. A

considerable part of the driving force for the reactions is therefore the displacement of equil. by pptn. The products in most cases are obtained in reasonable, and sometimes very high, yields after a reaction time of a few days, and are isolated in pure form directly from the reaction mixt., the usual losses thus being eliminated. Several of the reactions may have preparative value or may serve for future kinetic investigations. Some of the exptl. results support the theory that some reactions, normally considered to be base-catalyzed, may also take place under acid conditions. The following solubilities in H<sub>2</sub>O at approx. 18.degree. (g./100 g.) are reported: p-MeOC<sub>6</sub>H<sub>4</sub>CHO 0.38, p-HOC<sub>6</sub>H<sub>4</sub>CHO 0.81, PhCH:CHCHO 0.14, 1-ClOH<sub>7</sub>CHO 0.14, o-C<sub>6</sub>H<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub> (I) 2.16. Details are given (in tables) of the following reactions at various pH (time at room temp. given). PhCH:NPh from BzH and PhNH<sub>2</sub> (2 days): 80% at pH 7-7.9, 0% at pH 3.8. 2,3-Dimethylquinoxaline from I and Ac<sub>2</sub> (1 day): 81-98% at pH 4-9, 44% at pH 3, 82% at pH 11.6. 5,7-Dimethyl-2,3-benzo-1,4-diazepine from I and CH<sub>2</sub>Ac<sub>2</sub> (2 hrs.): 56% at pH 5.8, 0% at pH 8.2; HCl salt ppts. at pH 3.8. 2-Amino-4,6-dimethylpyrimidine from (H<sub>2</sub>N)<sub>2</sub>C:NH.H<sub>2</sub>CO<sub>3</sub> and CH<sub>2</sub>Ac<sub>2</sub> (20 days): 62% at pH 10, 0% at pH 8.5. 4,6-Dimethyl-2-phenylpyrimidine from PhC:(NH)NH<sub>2</sub> (19 days): 64% at pH 9.6, 36% at pH 9.1, 26% at pH 8.9, 8% at pH 8.7, 0% at pH 7.5 or below. Benzimidazole from I and HCO<sub>2</sub>H (5 days): 83% at pH 0.5, 25% at pH 2.3, 0% at pH 3.3. 4,6-Diamino-5-formamidopyrimidine (II) from 4,5,6-triaminopyrimidine (III) and HCO<sub>2</sub>H (4 days): 61% at pH 1.1, 3% at pH 2.8 or 0.3, 0% at 3.0 or above; adenine could not be detected but was formed by heating II 4 hrs. at 230.degree.; II was not cyclized (7 days at room temp.) at pH 11 or above (at pH 14 III was regenerated). (Furfurylideneacetyl)acetone (IV), m. 55-7.degree., at pH 4 results in 17% yield from furfuraldehyde (V) and CH<sub>2</sub>Ac<sub>2</sub> in 3 days and in 67% yield after 14 days; IV results (6 days) in 60-76% yield in the pH range 3.6-6.5; in the presence of 2 g. glycine (0.96 g. V), the yield is 92% (pH 4.7 (17% without catalyst); 0.1 g. glycine gives 56% and 1 g. gives 83%. 4-Cyanomethylimino-2-pentanone, m. 112-13.degree. (from H<sub>2</sub>NCH<sub>2</sub>CN and CH<sub>2</sub>Ac<sub>2</sub>) (8 days) results in 67-9% yields at pH 6.9-8.0; HO<sub>2</sub>CCH<sub>2</sub>N:CMech<sub>2</sub>Ac (from H<sub>2</sub>NCH<sub>2</sub>CO<sub>2</sub>Et and CH<sub>2</sub>Ac<sub>2</sub>) (2 days) is formed in 46-8% yield at pH 8.3-8.7, 0% at pH 7.1 or 9.0. 1-Benzyl-2,5-dimethylpyrrole (from PhCH<sub>2</sub>NH<sub>2</sub> and CH<sub>2</sub>Ac<sub>2</sub>) (7 days) results in 68-70% yield at pH 10.9-11.5, 1% at pH 7.1, and 0% at pH 5.8 or below. 2,5-Dimethyl-1-phenylpyrrole (from PhNH<sub>2</sub> and CH<sub>2</sub>Ac<sub>2</sub>) (8 days) results in 70% yield at pH 4.4 or 5.5, 0% above pH 8.2. Et 2-methyl-4-phenyl-3-pyrrolicarboxylate (from BzCH<sub>2</sub>NH<sub>2</sub> and AcCH<sub>2</sub>CO<sub>2</sub>Et) (3 days) results in 63% yield at pH 6.9-8.2, 14% at pH 6.1, and 2% at pH 3.9. 3-Cyano-4,6-dimethyl-2-pyridone (from NCCH<sub>2</sub>CONH<sub>2</sub> and CH<sub>2</sub>Ac<sub>2</sub>) (1 day) results in 74% yield at pH 9.1 and 20% at pH 6.4; in another expt., with K<sub>2</sub>CO<sub>3</sub> (1 day), the yield was 94-6% at pH 8.5-9.1, 0% at pH 4.4, 20% at pH 6.4. Di-Et 1,4-dihydrocollidine-3,5-dicarboxylate (from AcH, AcCH<sub>2</sub>CO<sub>2</sub>Et, and NH<sub>3</sub>) (4 days) results in 43% yield at pH 8.5 and 3% at pH 6. 3,5-Diacetyl-1,4-dihydrocollidine (from AcH, CH<sub>2</sub>Ac<sub>2</sub>, and NH<sub>3</sub>) (4 days) is formed in 23-9% yield at pH 6.3-9.0; with (NH<sub>4</sub>)<sub>2</sub>CO<sub>3</sub> the reaction is slower but the yield at pH 8.1 is 51%.

=&gt; d cost

COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
CONNECT CHARGES	1.36	1.85
NETWORK CHARGES	0.24	0.36
SEARCH CHARGES	1.64	149.39
DISPLAY CHARGES	43.20	43.20
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	46.44	194.80

10077150.3

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